Isobutyric anhydride 97-72-3 | DTXSID7026609

Model Performance

Marada I	D. L.
Model	Data
110001	Bata

Weighted KNN model

5-fold CV (5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.89	0.25	0.88	0.26	0.75	0.38	

Model Results

Predicted value: 5.65 days

Global applicability domain: Inside

Local applicability domain index: 3.87e-01

Confidence level: 8.21e-01

Nearest Neighbors from the Training Set

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Pentane

Measured: 40.7 **Predicted:** 6.52

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n-Hexane

Measured: 157 Predicted: 7.45

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Heptane

Measured: 88.3 Predicted: 7.54

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2-Methylhexane Measured: 12.5 Predicted: 5.54 Image not found

2,2-Dimethylheptane Measured: 61.9 Predicted: 5.05